

HYDROGEN BONDING IN THE MONOHYDRATED COMPLEXES OF TRIMETHYLENE OXIDE, SULFIDE AND SELENIDE: A ROTATIONAL SPECTROSCOPIC AND THEORETICAL INVESTIGATION

WESLLEY G. D. P. SILVA, JENNIFER VAN WIJNGAARDEN, *Department of Chemistry, University of Manitoba, Winnipeg, MB, Canada.*

The monohydrated complexes of trimethylene oxide and sulfide were investigated in the gas phase using Fourier transform microwave spectroscopy (8-18 GHz) aided by quantum mechanical calculations. In the assigned trimethylene oxide-water complex, the water subunit binds exclusively to the oxygen atom of the ring via a OH...O hydrogen bond (HB). In the sulfur containing complex, in addition to the primary OH...S HB, a secondary CH...O interaction is observed. The experimental results for the sulfur analog are consistent with the predictions from both *ab initio* and density functional theory (DFT) calculations with the aug-cc-pVTZ basis set whereas for the oxygen analog, both planar and puckered ring configurations are possible depending on the level of theory. Our experimental data aligns better with the results from DFT calculations which predict the trimethylene oxide ring to adopt a planar configuration in the complex. The nature and strength of the HBs are studied in detail using topological and energy decomposition analyses. Comparisons are also made computationally with the selenium analog to evaluate the characteristics of the HB along the chalcogen series. The results show that the HBs formed by these rings with water are mostly electrostatic and dispersive in nature and that the HB strength decreases from oxygen to selenium.